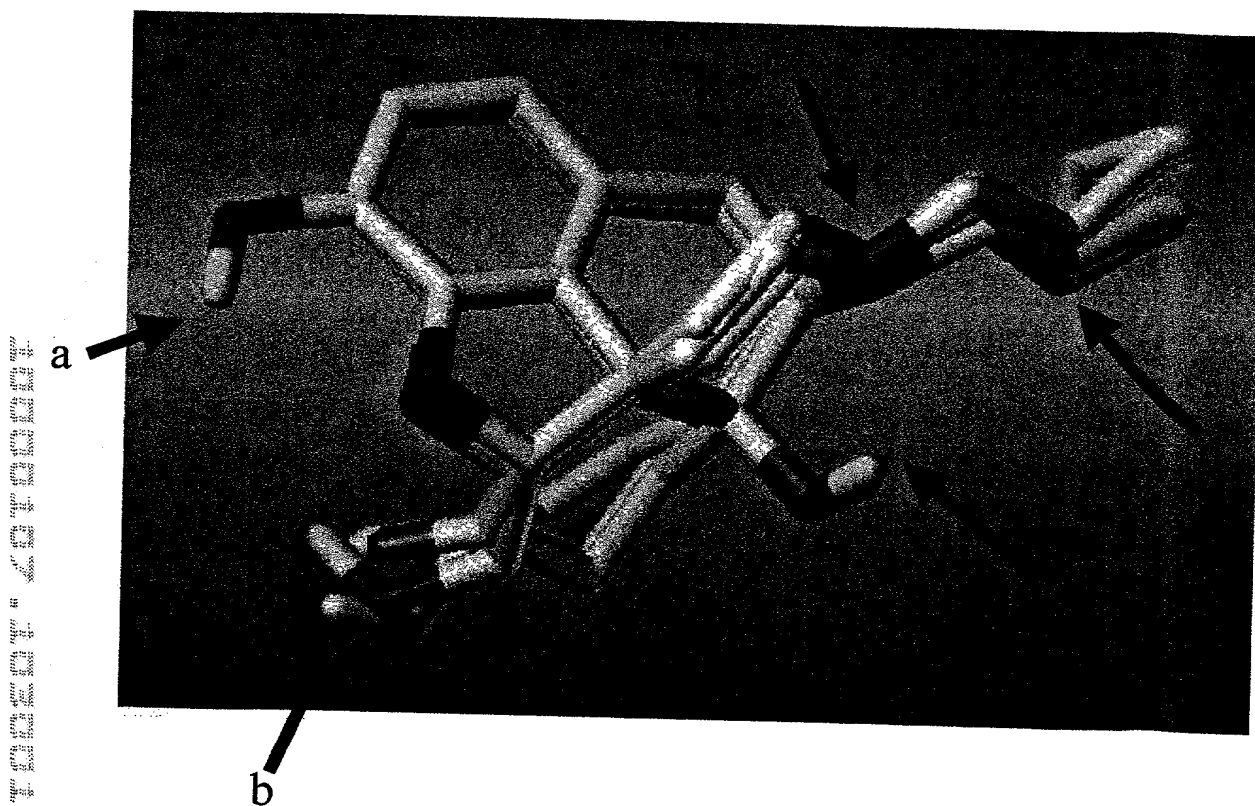
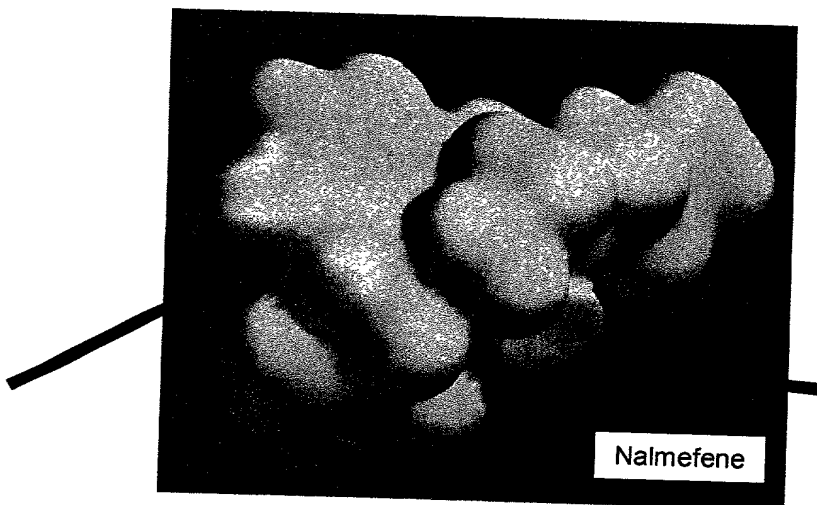
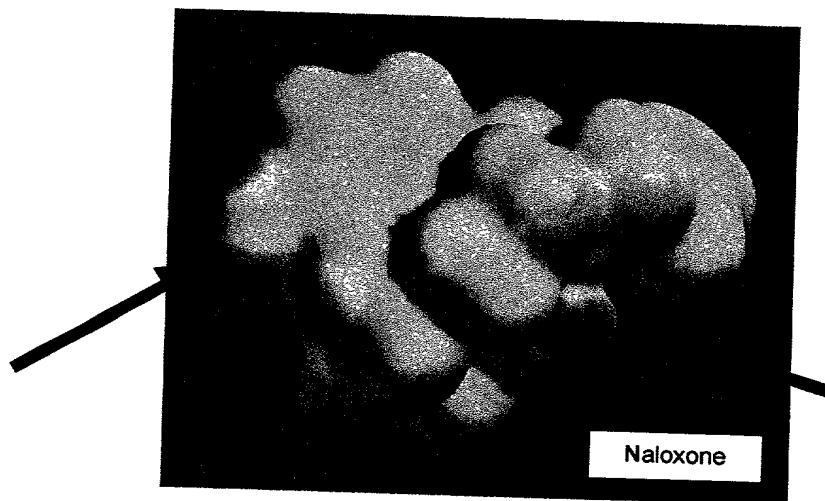


FIG. 1

**FIG. 2**



**FIG. 3A**



**FIG. 3B**

## 200 Neighbors

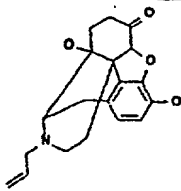
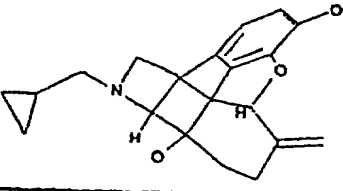
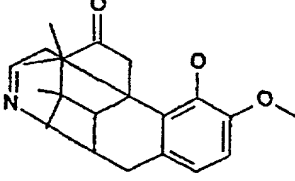
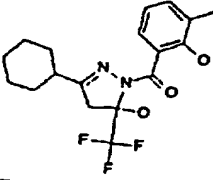
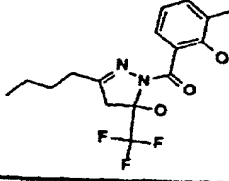
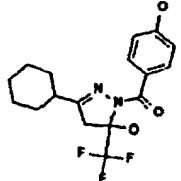
| Structure   | Cpd ID       |                         | MW      | Distance | Neighbor  |
|---|--------------|-------------------------|---------|----------|-----------|
|    | 70413        | $C_{19}H_{21}NO_4$      | 327.384 | 0.010    | Naloxone  |
|    | MFCD00133650 | $C_{21}H_{25}NO_3$      | 339.438 | 0.018    | Nalmefene |
|    | 349115       | $C_{21}H_{27}NO_3$      | 341.454 | 0.406    | Nalmefene |
|   | BAS 3387173  | $C_{18}H_{21}F_3N_2O_3$ | 370.375 | 0.510    | Naloxone  |
|  | BAS 1002455  | $C_{16}H_{19}F_3N_2O_3$ | 344.337 | 0.519    | Naloxone  |
|  | BAS 3387155  | $C_{17}H_{19}F_3N_2O_3$ | 356.348 | 0.524    | Naloxone  |
|   |              |                         |         |          |           |

Fig. 4A

## 200 Neighbors

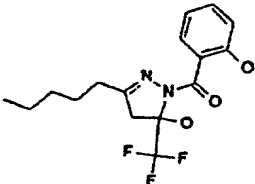
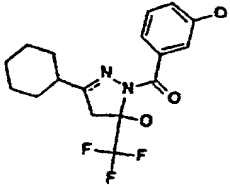
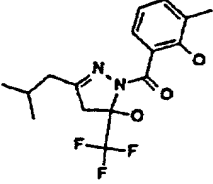
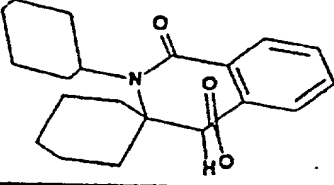
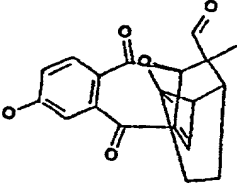
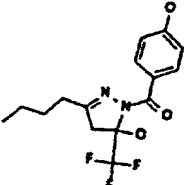
| Structure   | Cpd ID       |                         | MW      | Distance | Neighbor         |
|---|--------------|-------------------------|---------|----------|------------------|
|    | BAS 1268016  | $C_{16}H_{19}F_3N_2O_3$ | 344.337 | 0.534    | Naloxone         |
|    | BAS 3387156  | $C_{17}H_{19}F_3N_2O_3$ | 356.348 | 0.541    | Naloxone         |
|    | BAS 3387130  | $C_{16}H_{19}F_3N_2O_3$ | 344.337 | 0.546    | Naloxone         |
|   | MFCD01935543 | $C_{21}H_{27}NO_3$      | 341.454 | 0.551    | Naloxone         |
|  | 688277       | $C_{20}H_{18}O_5$       | 338.363 | 0.591    | 6-beta-Naltrexol |
|  | BAS 1002441  | $C_{15}H_{17}F_3N_2O_3$ | 330.310 | 0.618    | Naloxone         |
|   |              |                         |         |          |                  |

Fig. 4B

## 200 Neighbors

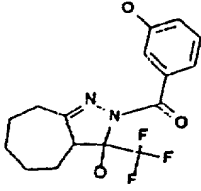
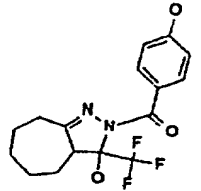
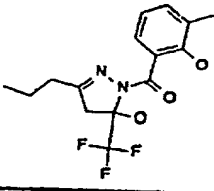
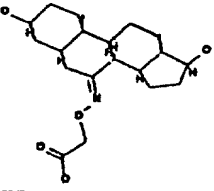
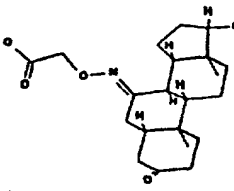
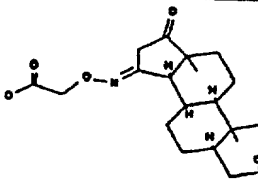
| Structure   | Cpd ID       |                         | MW      | Distance | Neighbor  |
|---|--------------|-------------------------|---------|----------|-----------|
|    | BAS 3386059  | $C_{16}H_{17}F_3N_2O_3$ | 342.321 | 0.637    | Naloxone  |
|    | BAS 1003176  | $C_{16}H_{17}F_3N_2O_3$ | 342.321 | 0.637    | Naloxone  |
|    | BAS 1004848  | $C_{15}H_{17}F_3N_2O_3$ | 330.310 | 0.643    | Naloxone  |
|   | MFCD00273259 | $C_{21}H_{33}NO_5$      | 379.501 | 0.644    | Nalmefene |
|  | MFCD00273270 | $C_{21}H_{31}NO_5$      | 377.485 | 0.646    | Naloxone  |
|  | MFCD00273266 | $C_{21}H_{31}NO_5$      | 377.485 | 0.648    | Naloxone  |
|   |              |                         |         |          |           |

Fig. 4C

## 200 Neighbors

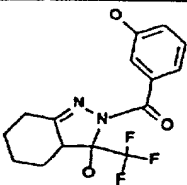
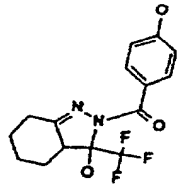
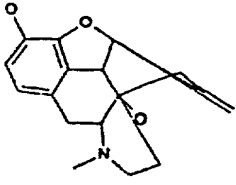
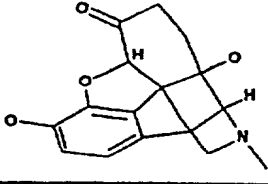
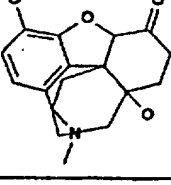
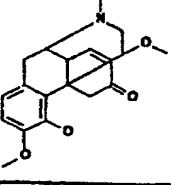
| Structure   | Cpd ID       |                         | MW      | Distance | Neighbor         |
|---|--------------|-------------------------|---------|----------|------------------|
|    | BAS 3386023  | $C_{15}H_{15}F_3N_2O_3$ | 328.294 | 0.653    | Naloxone         |
|    | BAS 2028128  | $C_{15}H_{15}F_3N_2O_3$ | 328.294 | 0.657    | Naloxone         |
|    | 617005       | $C_{18}H_{21}NO_3$      | 299.373 | 0.658    | 6-beta-Naltrexol |
|   | MFCD00079194 | $C_{17}H_{19}NO_4$      | 301.345 | 0.662    | 6-beta-Naltrexol |
|  | 19045        | $C_{17}H_{19}NO_4$      | 301.345 | 0.666    | 6-beta-Naltrexol |
|  | 76021        | $C_{19}H_{23}NO_4$      | 329.399 | 0.673    | Nalmefene        |
|   |              |                         |         |          |                  |

Fig. 4D

## 200 Neighbors

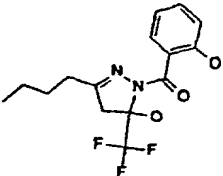
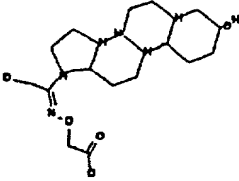
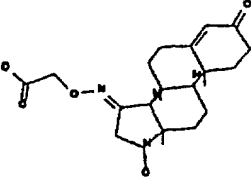
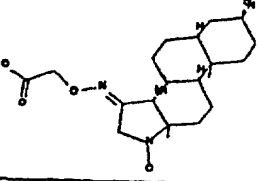
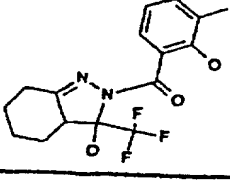
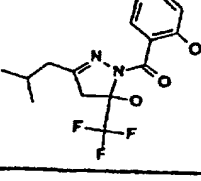
| Structure   | Cpd ID       |                         | MW      | Distance | Neighbor  |
|---|--------------|-------------------------|---------|----------|-----------|
|    | BAS 1002442  | $C_{15}H_{17}F_3N_2O_3$ | 330.310 | 0.677    | Naloxone  |
|    | MFCD00271723 | $C_{23}H_{37}NO_5$      | 407.555 | 0.682    | Naloxone  |
|    | MFCD00273273 | $C_{21}H_{29}NO_5$      | 375.469 | 0.688    | Nalmefene |
|   | MFCD00273264 | $C_{21}H_{33}NO_5$      | 379.501 | 0.697    | Nalmefene |
|  | BAS 2026145  | $C_{16}H_{17}F_3N_2O_3$ | 342.321 | 0.698    | Naloxone  |
|  | BAS 3387114  | $C_{15}H_{17}F_3N_2O_3$ | 330.310 | 0.704    | Naloxone  |
|   |              |                         |         |          |           |

Fig. 4E



## 200 Neighbors

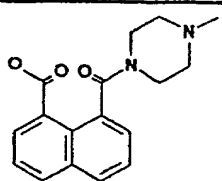
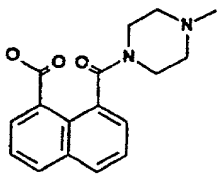
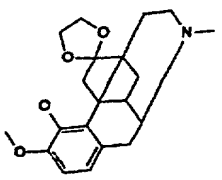
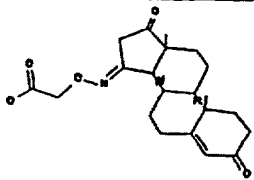
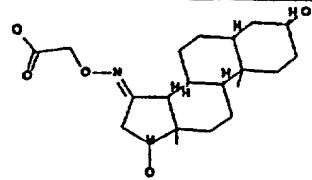
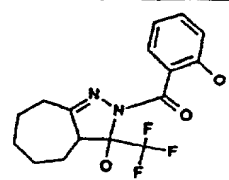
| Structure   | Cpd ID       |                         | MW      | Distance | Neighbor   |
|---|--------------|-------------------------|---------|----------|------------|
|    | 376679       | $C_{17}H_{18}N_2O_3$    | 298.345 | 0.705    | Naltrexone |
|    | 379963       | $C_{17}H_{18}N_2O_3$    | 298.345 | 0.705    | Naltrexone |
|    | 157870       | $C_{20}H_{27}NO_4$      | 345.442 | 0.714    | Nalmefene  |
|   | MFCD00273274 | $C_{21}H_{27}NO_5$      | 373.453 | 0.720    | Naloxone   |
|  | MFCD00273260 | $C_{21}H_{33}NO_5$      | 379.501 | 0.723    | Nalmefene  |
|  | BAS 1003163  | $C_{16}H_{17}F_3N_2O_3$ | 342.321 | 0.727    | Naloxone   |
|   |              |                         |         |          |            |

Fig. 4F

## 200 Neighbors

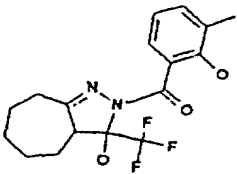
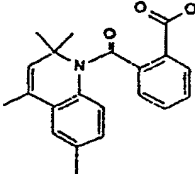
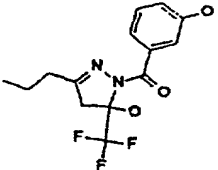
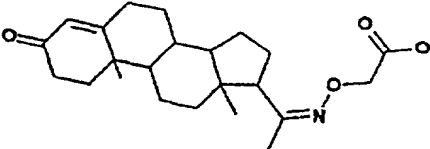
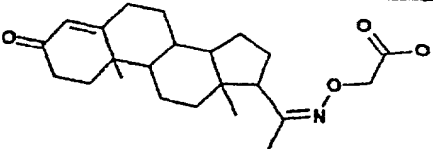
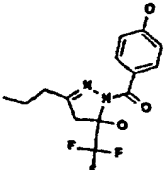
| Structure   | Cpd ID      |                         | MW      | Distance | Neighbor   |
|---|-------------|-------------------------|---------|----------|------------|
|    | BAS 1003182 | $C_{17}H_{19}F_3N_2O_3$ | 356.348 | 0.739    | Naltrexone |
|    | BAS 0510629 | $C_{21}H_{21}NO_3$      | 335.406 | 0.756    | Naltrexone |
|    | BAS 1002419 | $C_{14}H_{15}F_3N_2O_3$ | 316.282 | 0.757    | Naloxone   |
|   | 18579       | $C_{23}H_{33}NO_4$      | 387.524 | 0.760    | Nalmefene  |
|  | 58796       | $C_{23}H_{33}NO_4$      | 387.524 | 0.760    | Nalmefene  |
|  | BAS 1004835 | $C_{14}H_{15}F_3N_2O_3$ | 316.282 | 0.763    | Naloxone   |
|   |             |                         |         |          |            |

Fig. 4G

## 200 Neighbors

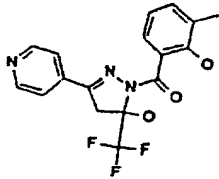
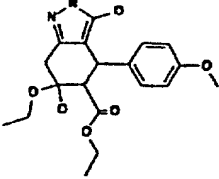
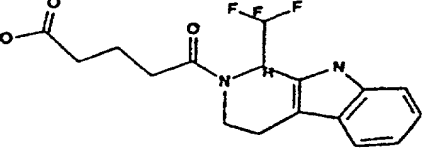
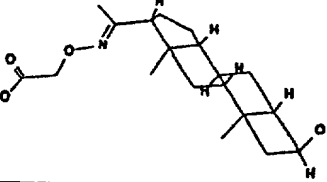
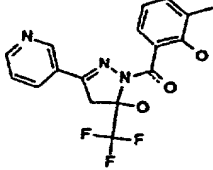
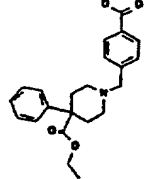
| Structure   | Cpd ID       |                         | MW      | Distance | Neighbor  |
|---|--------------|-------------------------|---------|----------|-----------|
|    | BAS 2004373  | $C_{17}H_{14}F_3N_3O_3$ | 365.315 | 0.765    | Naloxone  |
|    | 693856       | $C_{19}H_{24}N_2O_6$    | 376.413 | 0.768    | Nalmefene |
|    | MFCD01764789 | $C_{17}H_{17}F_3N_2O_3$ | 354.332 | 0.769    | Naloxone  |
|   | MFCD00271738 | $C_{23}H_{37}NO_4$      | 391.558 | 0.772    | Nalmefene |
|  | BAS 2025996  | $C_{17}H_{14}F_3N_3O_3$ | 365.315 | 0.774    | Naloxone  |
|  | BAS 2282169  | $C_{22}H_{25}NO_4$      | 367.449 | 0.780    | Nalmefene |
|   |              |                         |         |          |           |

Fig. 4H

## 200 Neighbors

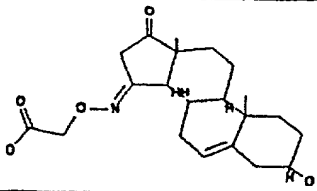
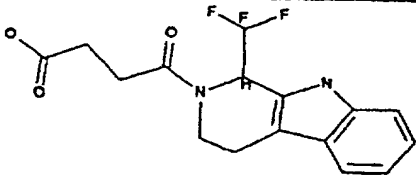
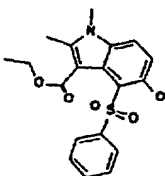
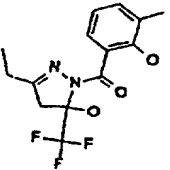
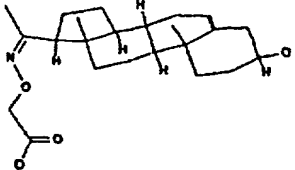
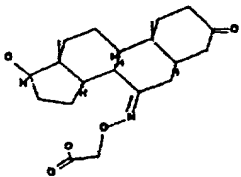
| Structure   | Cpd ID       |                         | MW      | Distance | Neighbor         |
|---|--------------|-------------------------|---------|----------|------------------|
|    | MFCD00273288 | $C_{21}H_{29}NO_5$      | 375.469 | 0.789    | Naloxone         |
|    | MFCD00179880 | $C_{16}H_{15}F_3N_2O_3$ | 340.305 | 0.800    | Naloxone         |
|    | BAS 1507170  | $C_{19}H_{19}NO_5S$     | 373.431 | 0.801    | Nalmefene        |
|   | BAS 3386088  | $C_{14}H_{15}F_3N_2O_3$ | 316.282 | 0.802    | Naloxone         |
|  | MFCD00272082 | $C_{23}H_{35}NO_4$      | 389.540 | 0.818    | Nalmefene        |
|  | MFCD00271113 | $C_{21}H_{31}NO_5$      | 377.485 | 0.829    | 6-beta-Naltrexol |
|   |              |                         |         |          |                  |

Fig. 4I

## 200 Neighbors

| Structure | Cpd ID       |                         | MW      | Distance | Neighbor         |
|-----------|--------------|-------------------------|---------|----------|------------------|
|           | 116054       | $C_{18}H_{19}N_3O_4$    | 341.370 | 0.831    | 6-beta-Naltrexol |
|           | BAS 1004837  | $C_{14}H_{15}F_3N_2O_3$ | 316.282 | 0.835    | Naloxone         |
|           | 134536       | $C_{19}H_{25}NO_3$      | 315.416 | 0.836    | 6-beta-Naltrexol |
|           | 615801       | $C_{17}H_{20}N_2O_3$    | 300.361 | 0.856    | Naltrexone       |
|           | 404374       | $C_{20}H_{27}NO_3$      | 329.443 | 0.870    | Nalmefene        |
|           | MFCD00273318 | $C_{23}H_{35}NO_4$      | 389.540 | 0.870    | Nalmefene        |

Fig. 4J

## 200 Neighbors

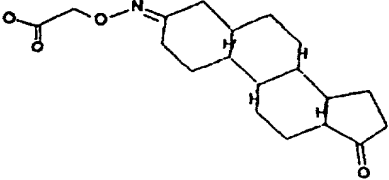
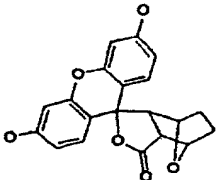
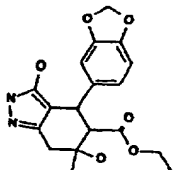
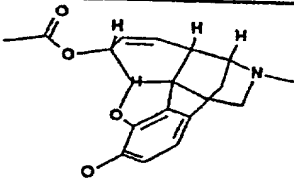
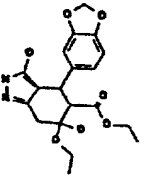
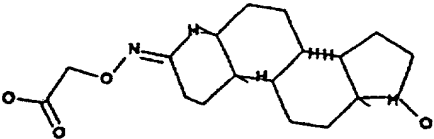
| Structure   | Cpd ID       |                      | MW      | Distance | Neighbor   |
|---|--------------|----------------------|---------|----------|------------|
|    | MFCD00271094 | $C_{21}H_{31}NO_4$   | 361.486 | 0.877    | Nalmefene  |
|    | 202587       | $C_{20}H_{16}O_6$    | 352.347 | 0.889    | Nalmefene  |
|    | 693862       | $C_{18}H_{20}N_2O_6$ | 360.370 | 0.892    | Nalmefene  |
|   | MFCD00467140 | $C_{19}H_{21}NO_4$   | 327.384 | 0.905    | Nalmefene  |
|  | 693863       | $C_{19}H_{22}N_2O_7$ | 390.396 | 0.909    | Naltrexone |
|  | MFCD00271196 | $C_{21}H_{33}NO_4$   | 363.501 | 0.912    | Nalmefene  |
|   |              |                      |         |          |            |

Fig. 4K

## 200 Neighbors

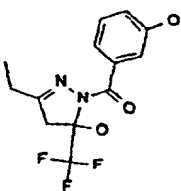
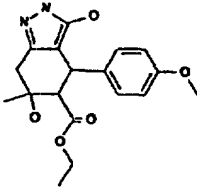
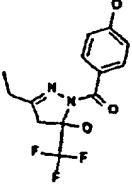
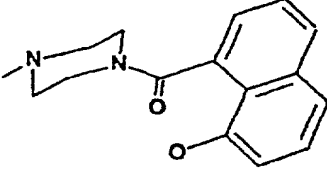
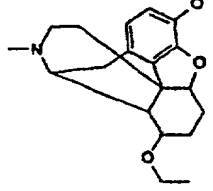
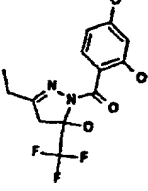
| Structure   | Cpd ID       |                         | MW      | Distance | Neighbor         |
|---|--------------|-------------------------|---------|----------|------------------|
|    | BAS 3386092  | $C_{13}H_{13}F_3N_2O_3$ | 302.255 | 0.919    | Naloxone         |
|    | 693855       | $C_{18}H_{22}N_2O_5$    | 348.386 | 0.923    | Nalmefene        |
|    | BAS 3386091  | $C_{13}H_{13}F_3N_2O_3$ | 302.255 | 0.928    | Naloxone         |
|   | MFCD00665833 | $C_{16}H_{18}N_2O_2$    | 270.334 | 0.929    | Naltrexone       |
|  | 404368       | $C_{19}H_{25}NO_3$      | 315.416 | 0.941    | 6-beta-Naltrexol |
|  | BAS 0606820  | $C_{13}H_{13}F_3N_2O_4$ | 318.255 | 0.948    | Naloxone         |
|   |              |                         |         |          |                  |

Fig. 4L

## 200 Neighbors

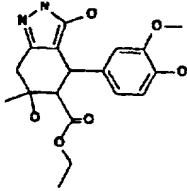
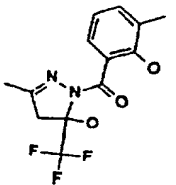
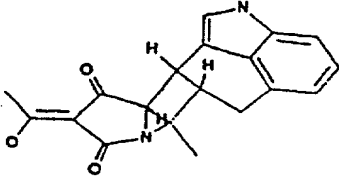
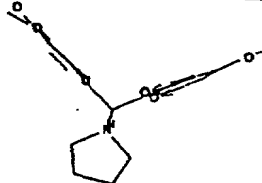
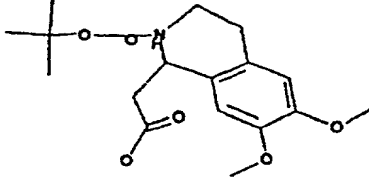
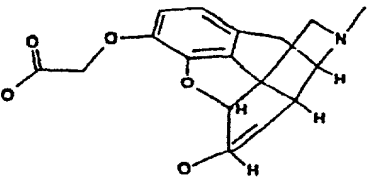
| Structure   | Cpd ID       |                         | MW      | Distance | Neighbor   |
|---|--------------|-------------------------|---------|----------|------------|
|    | 693859       | $C_{18}H_{22}N_2O_6$    | 362.388 | 0.849    | Nalmefene  |
|    | BAS 0436353  | $C_{13}H_{13}F_3N_2O_3$ | 302.255 | 0.965    | Naloxone   |
|    | MFCD00167445 | $C_{20}H_{20}N_2O_3$    | 336.394 | 0.968    | Naltrexone |
|   | MFCD00667402 | $C_{21}H_{25}NO_6$      | 387.437 | 0.974    | Nalmefene  |
|  | MFCD02258126 | $C_{18}H_{25}NO_6$      | 351.403 | 0.977    | Naloxone   |
|  | MFCD00143186 | $C_{19}H_{21}NO_5$      | 343.383 | 0.985    | Naltrexone |
|   |              |                         |         |          |            |

Fig. 4M



## 200 Neighbors

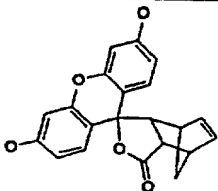
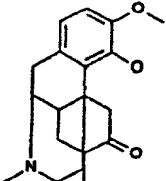
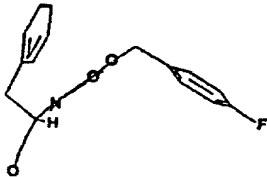
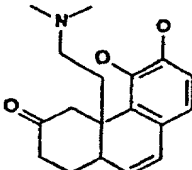
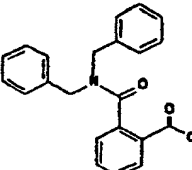
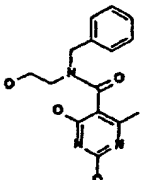
| Structure   | Cpd ID       |                      | MW      | Distance | Neighbor         |
|---|--------------|----------------------|---------|----------|------------------|
|    | 119887       | $C_{21}H_{16}O_5$    | 348.359 | 0.993    | Naloxone         |
|    | 404365       | $C_{19}H_{25}NO_3$   | 315.416 | 1.002    | Nalmefene        |
|    | MFCD01871411 | $C_{21}H_{20}FNO_3$  | 353.397 | 1.012    | Naloxone         |
|   | 152720       | $C_{18}H_{23}NO_3$   | 301.389 | 1.015    | 6-beta-Naltrexol |
|  | 117581       | $C_{22}H_{19}NO_3$   | 345.402 | 1.016    | Naloxone         |
|  | 669466       | $C_{15}H_{17}N_3O_4$ | 303.320 | 1.017    | Naloxone         |
|   |              |                      |         |          |                  |

Fig. 4N

## 200 Neighbors

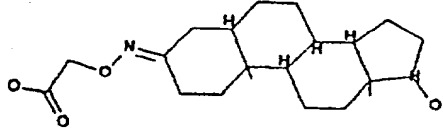
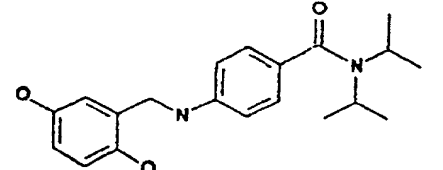
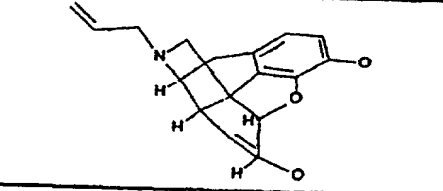
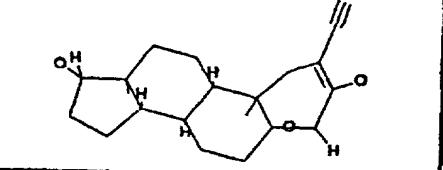
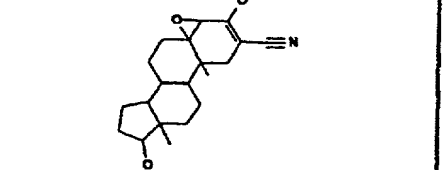
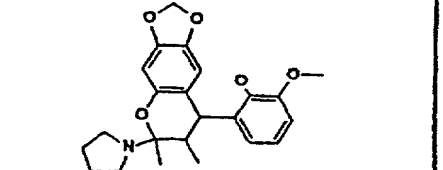
| Structure   | Cpd ID       |                      | MW      | Distance | Neighbor         |
|---|--------------|----------------------|---------|----------|------------------|
|    | MFCD00271129 | $C_{21}H_{33}NO_4$   | 363.501 | 1.029    | Nalmefene        |
|    | 689431       | $C_{20}H_{26}N_2O_3$ | 342.442 | 1.035    | 6-beta-Naltrexol |
|    | MFCD00056772 | $C_{19}H_{21}NO_3$   | 311.384 | 1.039    | Nalmefene        |
|   | MFCD00199295 | $C_{20}H_{27}NO_3$   | 329.443 | 1.045    | Nalmefene        |
|  | R191469      | $C_{20}H_{27}NO_3$   | 329.443 | 1.046    | Nalmefene        |
|  | 375504       | $C_{23}H_{27}NO_5$   | 397.475 | 1.050    | Naloxone         |
|   |              |                      |         |          |                  |

Fig. 40

## 200 Neighbors

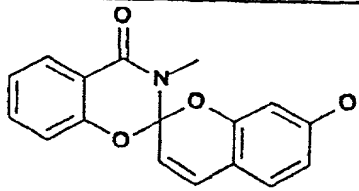
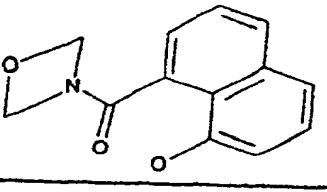
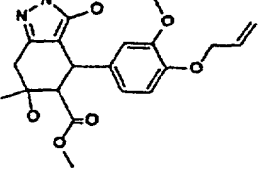
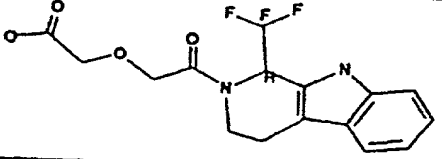
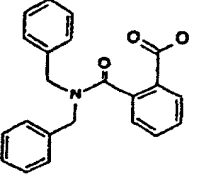
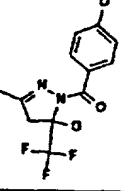
| Structure   | Cpd ID       |                         | MW      | Distance | Neighbor  |
|---|--------------|-------------------------|---------|----------|-----------|
|    | 692397       | $C_{17}H_{13}NO_4$      | 295.297 | 1.066    | Naloxone  |
|    | MFCD00433684 | $C_{15}H_{15}NO_3$      | 257.292 | 1.069    | Naloxone  |
|    | 693860       | $C_{20}H_{24}N_2O_6$    | 388.424 | 1.071    | Nalmefene |
|   | MFCD01764791 | $C_{16}H_{15}F_3N_2O_4$ | 356.304 | 1.073    | Naloxone  |
|  | BAS 1519270  | $C_{22}H_{19}NO_3$      | 345.402 | 1.078    | Naloxone  |
|  | BAS 3385849  | $C_{12}H_{11}F_3N_2O_3$ | 288.228 | 1.083    | Naloxone  |
|   |              |                         |         |          |           |

Fig. 4P

## 200 Neighbors

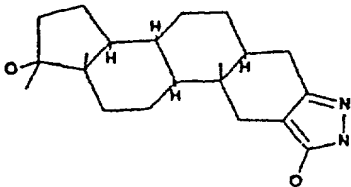
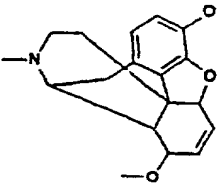
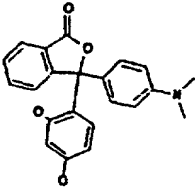
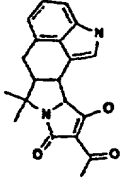
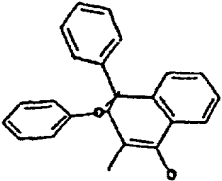
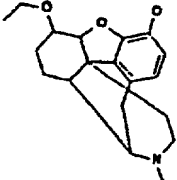
| Structure   | Cpd ID       |                      | MW      | Distance | Neighbor         |
|---|--------------|----------------------|---------|----------|------------------|
|    | MFCD00673308 | $C_{21}H_{32}N_2O_2$ | 344.501 | 1.087    | Nalmefene        |
|    | 404356       | $C_{18}H_{21}NO_3$   | 299.373 | 1.099    | Nalmefene        |
|    | 43938        | $C_{22}H_{19}NO_4$   | 361.401 | 1.107    | Nalmefene        |
|   | 117181       | $C_{20}H_{20}N_2O_3$ | 336.394 | 1.109    | Naltrexone       |
|  | MFCD00094379 | $C_{24}H_{22}O_2$    | 342.442 | 1.111    | Nalmefene        |
|  | 404369       | $C_{19}H_{25}NO_3$   | 315.416 | 1.111    | 6-beta-Naltrexol |
|   |              |                      |         |          |                  |

Fig. 4Q

## 200 Neighbors

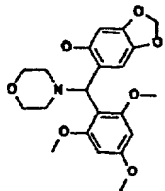
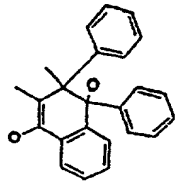
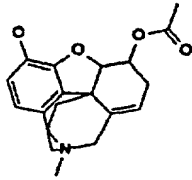
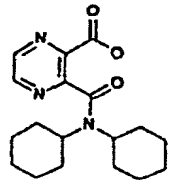
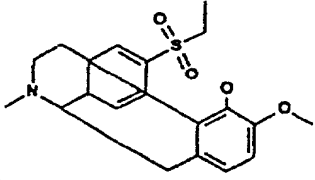
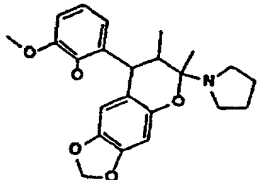
| Structure   | Cpd ID      |                      | MW      | Distance | Neighbor         |
|---|-------------|----------------------|---------|----------|------------------|
|    | 381577      | $C_{21}H_{25}NO_7$   | 403.436 | 1.111    | Naloxone         |
|    | S842214     | $C_{24}H_{22}O_2$    | 342.442 | 1.112    | Nalmefene        |
|    | 134602      | $C_{19}H_{21}NO_4$   | 327.384 | 1.112    | 6-beta-Naltrexol |
|   | CHS 0316796 | $C_{18}H_{25}N_3O_3$ | 331.418 | 1.113    | Naloxone         |
|  | 134604      | $C_{20}H_{25}NO_4S$  | 375.491 | 1.115    | Nalmefene        |
|  | R171697     | $C_{23}H_{27}NO_5$   | 397.475 | 1.133    | Nalmefene        |
|   |             |                      |         |          |                  |

Fig. 4R

## 200 Neighbors

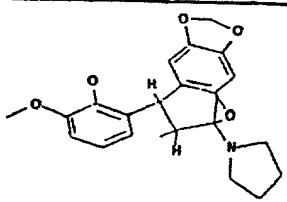
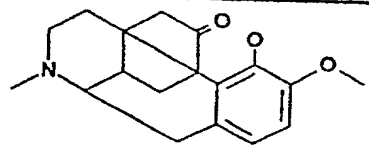
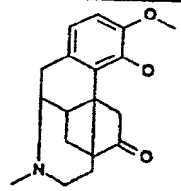
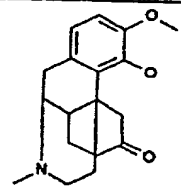
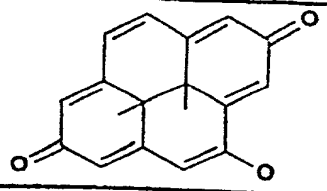
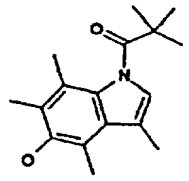
| Structure  | Cpd ID       |                      | MW      | Distance | Neighbor         |
|--|--------------|----------------------|---------|----------|------------------|
|     | MFCD00667401 | $C_{23}H_{27}NO_5$   | 397.475 | 1.134    | Nalmefene        |
|  Cl | S959863      | $C_{18}H_{24}ClNO_3$ | 337.850 | 1.137    | 6-beta-Naltrexol |
|     | 35545        | $C_{18}H_{23}NO_3$   | 301.389 | 1.137    | 6-beta-Naltrexol |
|    | 134598       | $C_{18}H_{23}NO_3$   | 301.389 | 1.137    | 6-beta-Naltrexol |
|   | S310778      | $C_{18}H_{14}O_3$    | 278.310 | 1.140    | Naloxone         |
|   | 669800       | $C_{17}H_{23}NO_2$   | 273.378 | 1.141    | Naloxone         |
|  |              |                      |         |          |                  |

Fig. 4S

## 200 Neighbors

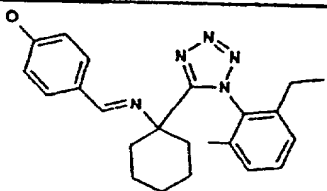
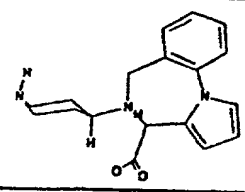
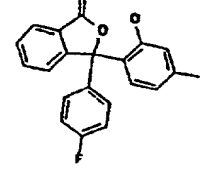
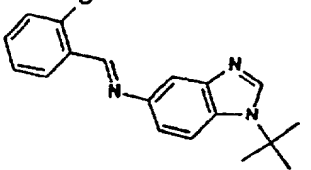
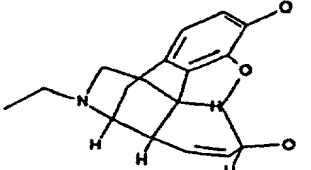
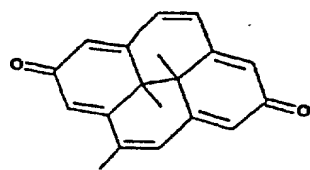
| Structure   | Cpd ID       |                      | MW      | Distance | Neighbor         |
|---|--------------|----------------------|---------|----------|------------------|
|    | BAS 0083962  | $C_{23}H_{27}N_5O$   | 389.505 | 1.141    | Naltrexone       |
|    | MFCD01765597 | $C_{18}H_{21}N_3O_2$ | 311.387 | 1.142    | 6-beta-Naltrexol |
|    | 682334       | $C_{21}H_{15}FO_3$   | 334.350 | 1.143    | Naloxone         |
|   | BAS 0631739  | $C_{18}H_{19}N_3O$   | 293.372 | 1.143    | Nalmefene        |
|  | MFCD00144882 | $C_{18}H_{21}NO_3$   | 299.373 | 1.149    | 6-beta-Naltrexol |
|  | MFCD00229975 | $C_{18}H_{14}O_3$    | 278.310 | 1.150    | Naloxone         |
|   |              |                      |         |          |                  |

Fig. 4T

## 200 Neighbors

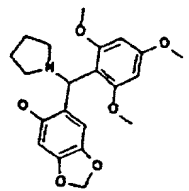
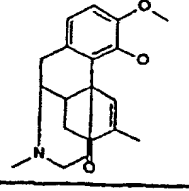
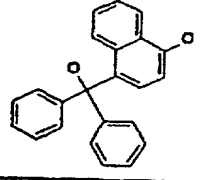
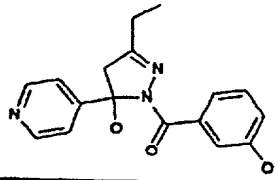
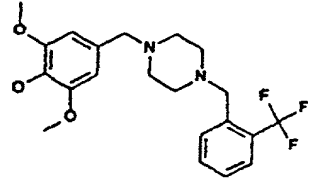
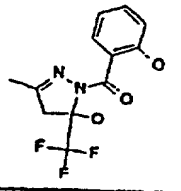
| Structure   | Cpd ID      |                         | MW      | Distance | Neighbor         |
|---|-------------|-------------------------|---------|----------|------------------|
|    | R171700     | $C_{21}H_{25}NO_6$      | 387.437 | 1.157    | Nalmefene        |
|    | 134592      | $C_{19}H_{23}NO_3$      | 313.400 | 1.163    | 6-beta-Naltrexol |
|    | 401210      | $C_{23}H_{18}O_2$       | 326.399 | 1.166    | Nalmefene        |
|   | BAS 2026074 | $C_{17}H_{17}N_3O_3$    | 311.343 | 1.172    | Naltrexone       |
|  | BAS 3050727 | $C_{21}H_{25}F_3N_2O_3$ | 410.440 | 1.177    | Nalmefene        |
|  | BAS 0341630 | $C_{12}H_{11}F_3N_2O_3$ | 288.228 | 1.185    | Naloxone         |
|   |             |                         |         |          |                  |

Fig. 4U



## 200 Neighbors

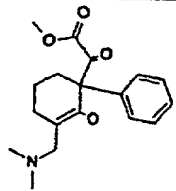
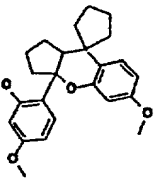
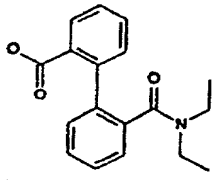
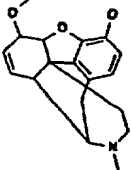
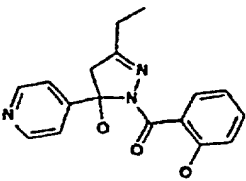
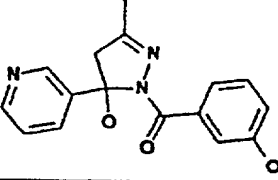
| Structure   | Cpd ID      |                      | MW      | Distance | Neighbor         |
|---|-------------|----------------------|---------|----------|------------------|
|    | 97817       | $C_{18}H_{23}NO_4$   | 317.388 | 1.190    | Naloxone         |
|    | ASN 3185453 | $C_{24}H_{28}O_4$    | 380.488 | 1.196    | Naloxone         |
|    | 21257       | $C_{18}H_{19}NO_3$   | 297.357 | 1.196    | 6-beta-Naltrexol |
|   | 134601      | $C_{18}H_{21}NO_3$   | 299.373 | 1.200    | 6-beta-Naltrexol |
|  | BAS 2026075 | $C_{17}H_{17}N_3O_3$ | 311.343 | 1.203    | 6-beta-Naltrexol |
|  | BAS 1996620 | $C_{16}H_{15}N_3O_3$ | 297.316 | 1.211    | 6-beta-Naltrexol |
|   |             |                      |         |          |                  |

Fig. 4V

## 200 Neighbors

| Structure | Cpd ID       |                         | MW      | Distance | Neighbor   |
|-----------|--------------|-------------------------|---------|----------|------------|
|           | MFCD01314358 | $C_{14}H_{14}F_3N_3O_3$ | 329.281 | 1.215    | Naloxone   |
|           | BAS 2026097  | $C_{18}H_{19}N_3O_3$    | 325.370 | 1.221    | Naltrexone |
|           | BAS 1914007  | $C_{21}H_{30}N_2O_3$    | 358.485 | 1.221    | Naloxone   |
|           | CHS 0003221  | $C_{16}H_{21}NO_3$      | 275.351 | 1.227    | Naloxone   |
|           | 667256       | $C_{20}H_{12}O_5$       | 332.316 | 1.227    | Naloxone   |
|           | 37625        | $C_{25}H_{20}O_2$       | 352.437 | 1.235    | Nalmefene  |
|           |              |                         |         |          |            |

Fig. 4W

## 200 Neighbors

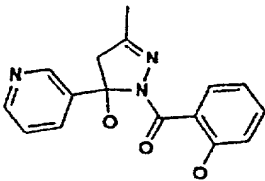
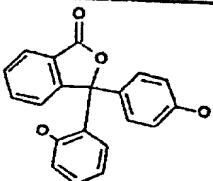
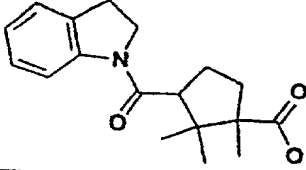
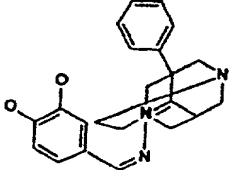
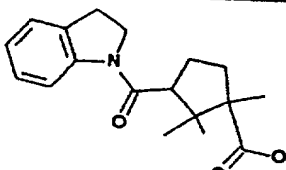
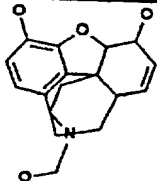
| Structure   | Cpd ID      |                      | MW      | Distance | Neighbor         |
|---|-------------|----------------------|---------|----------|------------------|
|    | BAS 1003093 | $C_{16}H_{15}N_3O_3$ | 297.316 | 1.236    | 6-beta-Naltrexol |
|    | 16468       | $C_{20}H_{14}O_4$    | 318.332 | 1.238    | Naloxone         |
|    | CHS 0227049 | $C_{18}H_{23}NO_3$   | 301.389 | 1.241    | Naloxone         |
|   | BAS 0315050 | $C_{22}H_{24}N_4O_2$ | 376.462 | 1.241    | Nalmefene        |
|  | BAS 1289763 | $C_{18}H_{23}NO_3$   | 301.389 | 1.242    | Naloxone         |
|  | 349127      | $C_{17}H_{19}NO_4$   | 301.345 | 1.243    | Naloxone         |
|   |             |                      |         |          |                  |

Fig. 4X

## 200 Neighbors

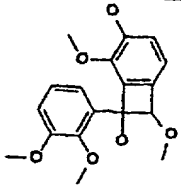
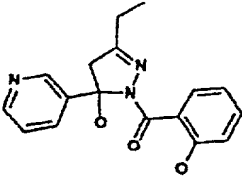
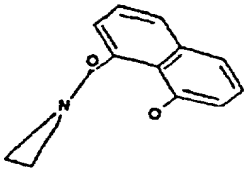
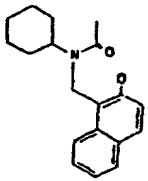
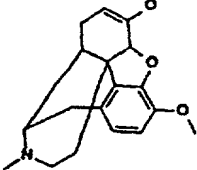
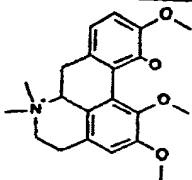
| Structure   | Cpd ID       |                      | MW      | Distance | Neighbor         |
|---|--------------|----------------------|---------|----------|------------------|
|    | 635928       | $C_{18}H_{20}O_6$    | 332.356 | 1.250    | Nalmefene        |
|    | BAS 2377555  | $C_{17}H_{17}N_3O_3$ | 311.343 | 1.251    | 6-beta-Naltrexol |
|    | MFCD00665835 | $C_{15}H_{15}NO_2$   | 241.292 | 1.251    | Naltrexone       |
|   | 47931        | $C_{19}H_{23}NO_2$   | 297.401 | 1.255    | 6-beta-Naltrexol |
|  | 76435        | $C_{18}H_{21}NO_3$   | 299.373 | 1.257    | Nalmefene        |
|  | 90558        | $C_{21}H_{26}NO_4$   | 356.446 | 1.258    | Naloxone         |
|   |              |                      |         |          |                  |

Fig. 4Y

## 200 Neighbors

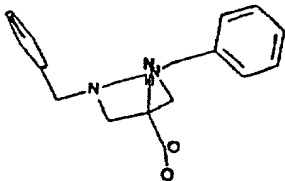
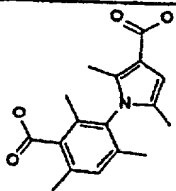
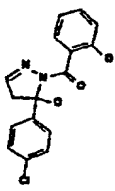
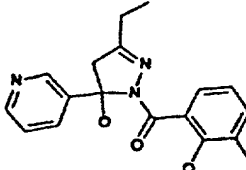
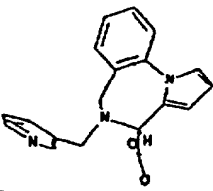
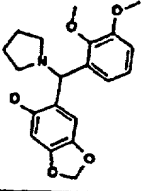
| Structure   | Cpd ID       |                        | MW      | Distance | Neighbor   |
|---|--------------|------------------------|---------|----------|------------|
|    | MFCD00206273 | $C_{20}H_{21}N_3O_2$   | 335.409 | 1.261    | Naloxone   |
|    | 159208       | $C_{17}H_{19}NO_4$     | 301.345 | 1.267    | Nalmefene  |
|    | BAS 0341580  | $C_{16}H_{13}ClN_2O_3$ | 316.747 | 1.267    | Naltrexone |
|   | BAS 2377575  | $C_{18}H_{19}N_3O_3$   | 325.370 | 1.268    | Naltrexone |
|  | MFCD01765638 | $C_{19}H_{17}N_3O_2$   | 319.366 | 1.268    | Nalmefene  |
|  | R171484      | $C_{20}H_{23}NO_5$     | 357.410 | 1.268    | Nalmefene  |
|   |              |                        |         |          |            |

Fig. 4Z

## 200 Neighbors

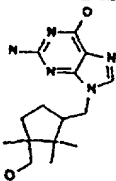
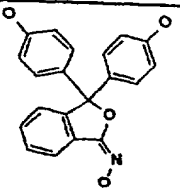
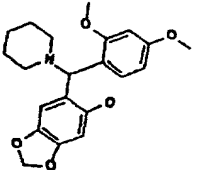
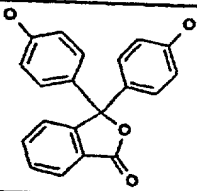
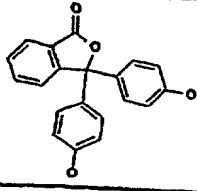
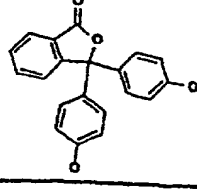
| Structure   | Cpd ID  |                    | MW      | Distance | Neighbor  |
|---|---------|--------------------|---------|----------|-----------|
|    | 700350  | $C_{15}H_{23}NO_2$ | 305.383 | 1.272    | Naloxone  |
|    | 16907   | $C_{20}H_{15}NO_4$ | 333.347 | 1.274    | Nalmefene |
|    | R170623 | $C_{21}H_{25}NO_5$ | 371.437 | 1.275    | Nalmefene |
|   | S98907  | $C_{20}H_{14}O_4$  | 318.332 | 1.278    | Naloxone  |
|  | 10464   | $C_{20}H_{14}O_4$  | 318.332 | 1.278    | Naloxone  |
|  | 215214  | $C_{20}H_{14}O_4$  | 318.332 | 1.278    | Naloxone  |
|   |         |                    |         |          |           |

Fig. 4AA

## 200 Neighbors

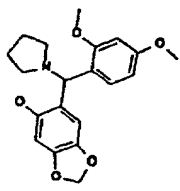
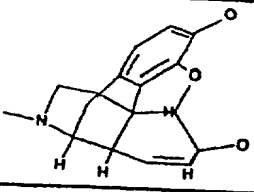
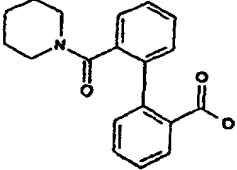
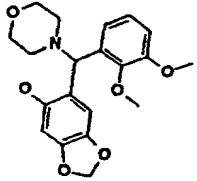
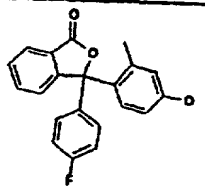
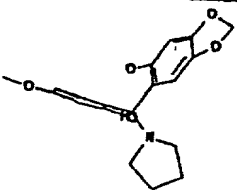
| Structure   | Cpd ID       |                    | MW      | Distance | Neighbor         |
|---|--------------|--------------------|---------|----------|------------------|
|    | R171425      | $C_{20}H_{23}NO_5$ | 357.410 | 1.280    | Nalmefene        |
|    | MFCD00153032 | $C_{17}H_{19}NO_3$ | 285.346 | 1.283    | 6-beta-Naltrexol |
|    | S196991      | $C_{19}H_{19}NO_3$ | 309.368 | 1.285    | Naltrexone       |
|   | R170291      | $C_{20}H_{23}NO_6$ | 373.409 | 1.286    | Naloxone         |
|  | 682335       | $C_{21}H_{15}FO_3$ | 334.350 | 1.287    | Naloxone         |
|  | MFCD00667377 | $C_{20}H_{23}NO_5$ | 357.410 | 1.289    | Nalmefene        |
|   |              |                    |         |          |                  |

Fig. 4AB

## 200 Neighbors

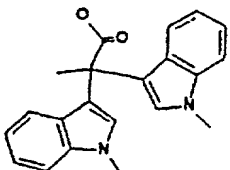
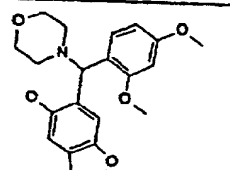
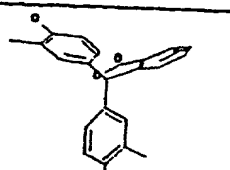
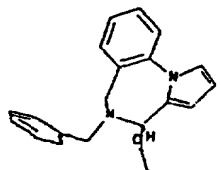
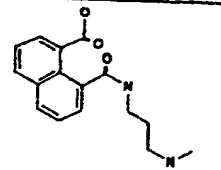
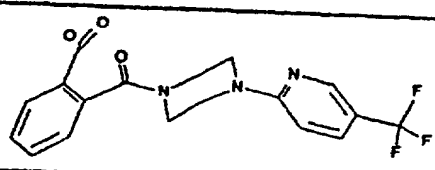
| Structure   | Cpd ID       |                         | MW      | Distance | Neighbor   |
|---|--------------|-------------------------|---------|----------|------------|
|    | 106242       | $C_{21}H_{20}N_2O_2$    | 332.408 | 1.294    | Naloxone   |
|    | R170410      | $C_{20}H_{23}NO_6$      | 373.409 | 1.299    | Naloxone   |
|    | MFCD00005912 | $C_{22}H_{18}O_4$       | 346.386 | 1.300    | Naloxone   |
|   | MFCD01765637 | $C_{20}H_{18}N_2O_2$    | 318.379 | 1.302    | Nalmefene  |
|  | 376678       | $C_{17}H_{20}N_2O_3$    | 300.361 | 1.303    | Naltrexone |
|  | MFCD01314431 | $C_{18}H_{16}F_3N_3O_3$ | 379.342 | 1.303    | Naloxone   |
|   |              |                         |         |          |            |

Fig. 4AC



## 200 Neighbors

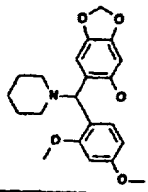
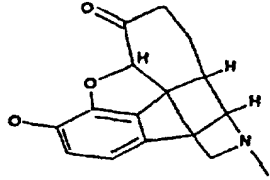
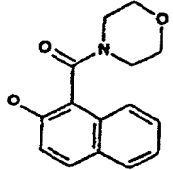
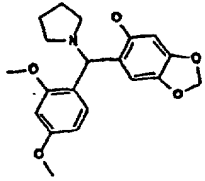
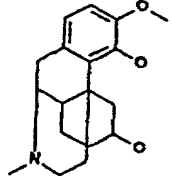
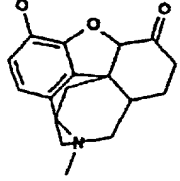
| Structure   | Cpd ID       |                    | MW      | Distance | Neighbor         |
|---|--------------|--------------------|---------|----------|------------------|
|    | 370278       | $C_{21}H_{25}NO_5$ | 371.437 | 1.304    | Nalmefene        |
|    | MFCD00242635 | $C_{17}H_{19}NO_3$ | 285.346 | 1.305    | 6-beta-Naltrexol |
|    | S602965      | $C_{15}H_{15}NO_3$ | 257.292 | 1.306    | Naltrexone       |
|   | 370279       | $C_{20}H_{23}NO_5$ | 357.410 | 1.306    | Nalmefene        |
|  | 157877       | $C_{18}H_{25}NO_3$ | 303.405 | 1.310    | Nalmefene        |
|  | 19046        | $C_{17}H_{19}NO_3$ | 285.346 | 1.310    | 6-beta-Naltrexol |
|   |              |                    |         |          |                  |

Fig. 4AD

## 200 Neighbors

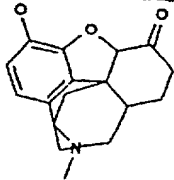
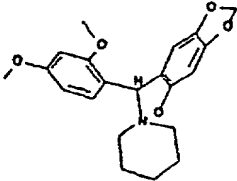
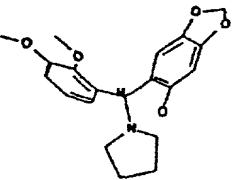
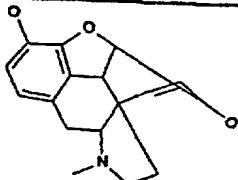
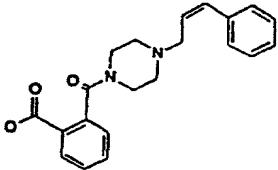
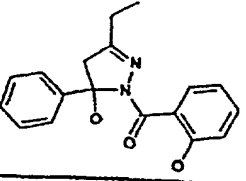
| Structure   | Cpd ID       |                      | MW      | Distance | Neighbor         |
|---|--------------|----------------------|---------|----------|------------------|
|    | 117862       | $C_{17}H_{19}NO_3$   | 285.348 | 1.310    | 6-beta-Naltrexol |
|    | MFCD00667305 | $C_{21}H_{25}NO_5$   | 371.437 | 1.313    | Nalmefene        |
|    | MFCD00667382 | $C_{20}H_{23}NO_5$   | 357.410 | 1.316    | Nalmefene        |
|   | 611276       | $C_{17}H_{19}NO_3$   | 285.346 | 1.318    | 6-beta-Naltrexol |
|  | BAS 1099232  | $C_{21}H_{22}N_2O_3$ | 350.421 | 1.320    | Naltrexone       |
|  | BAS 0313319  | $C_{18}H_{18}N_2O_3$ | 310.356 | 1.321    | 6-beta-Naltrexol |
|   |              |                      |         |          |                  |

Fig. 4AE

## 200 Neighbors

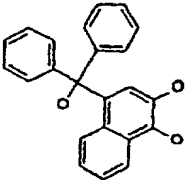
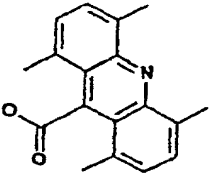
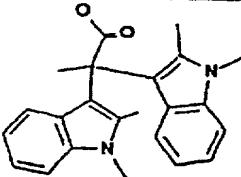
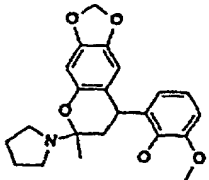
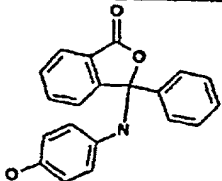
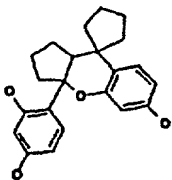
| Structure   | Cpd ID      |                      | MW      | Distance | Neighbor  |
|---|-------------|----------------------|---------|----------|-----------|
|    | 401211      | $C_{23}H_{18}O_3$    | 342.398 | 1.325    | Nalmefene |
|    | 409635      | $C_{18}H_{17}NO_2$   | 279.342 | 1.326    | Nalmefene |
|    | 106231      | $C_{23}H_{24}N_2O_2$ | 360.460 | 1.327    | Naloxone  |
|   | 375505      | $C_{22}H_{25}NO_5$   | 383.448 | 1.329    | Naloxone  |
|  | BAS 1053035 | $C_{20}H_{15}NO_3$   | 317.347 | 1.331    | Naloxone  |
|  | ASN 3160807 | $C_{22}H_{24}O_4$    | 352.434 | 1.332    | Naloxone  |
|   |             |                      |         |          |           |

Fig. 4AF

## 200 Neighbors

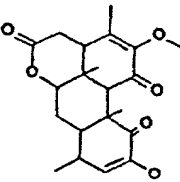
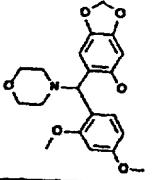
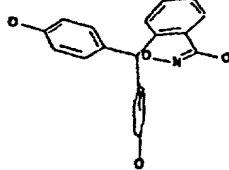
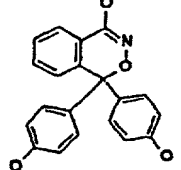
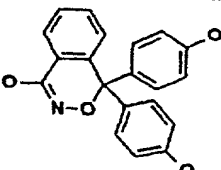
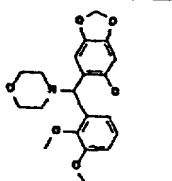
| Structure   | Cpd ID       |                    | MW      | Distance | Neighbor         |
|---|--------------|--------------------|---------|----------|------------------|
|    | 324633       | $C_{21}H_{26}O_6$  | 374.438 | 1.333    | Naloxone         |
|    | 370277       | $C_{20}H_{23}NO_8$ | 373.409 | 1.339    | Naloxone         |
|    | MFCD00375811 | $C_{20}H_{15}NO_4$ | 333.347 | 1.343    | 6-beta-Naltrexol |
|   | BAS 0659522  | $C_{20}H_{15}NO_4$ | 333.347 | 1.343    | 6-beta-Naltrexol |
|  | CHS 0305736  | $C_{20}H_{15}NO_4$ | 333.347 | 1.343    | 6-beta-Naltrexol |
|  | 381576       | $C_{20}H_{23}NO_6$ | 373.409 | 1.348    | Naloxone         |
|   |              |                    |         |          |                  |

Fig. 4AG

## 200 Neighbors

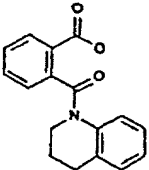
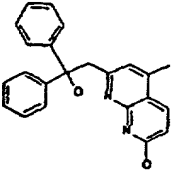
| Structure   | Cpd ID      |                      | MW      | Distance | Neighbor  |
|---|-------------|----------------------|---------|----------|-----------|
|  | CHS 0120289 | $C_{17}H_{15}NO_3$   | 281.314 | 1.348    | Naloxone  |
|  | 351159      | $C_{23}H_{20}N_2O_2$ | 356.428 | 1.349    | Nalmefene |
|   |             |                      |         |          |           |

Fig. 4AH